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Toward Automatic Model Comparison: An Adaptive Sequential Monte Carlo Approach

Yan ZHOU, Adam M. JOHANSEN, and John A.D. ASTON

Model comparison for the purposes of selection, averaging, and validation is a problem found throughout statistics. Within the Bayesian paradigm, these problems all require the calculation of the posterior probabilities of models within a particular class. Substantial progress has been made in recent years, but difficulties remain in the implementation of existing schemes. This article presents adaptive sequential Monte Carlo (SMC) sampling strategies to characterize the posterior distribution of a collection of models, as well as the parameters of those models. Both a simple product estimator and a combination of SMC and a path sampling estimator are considered and existing theoretical results are extended to include the path sampling variant. A novel approach to the automatic specification of distributions within SMC algorithms is presented and shown to outperform the state of the art in this area. The performance of the proposed strategies is demonstrated via an extensive empirical study. Comparisons with state-of-the-art algorithms show that the proposed algorithms are always competitive, and often substantially superior to alternative techniques, at equal computational cost and considerably less application-specific implementation effort. Supplementary materials for this article are available online.

Key Words: Adaptive Monte Carlo algorithms; Bayesian model comparison; Normalizing constants; Path sampling; Thermodynamic integration.

1. INTRODUCTION

Model comparison lies at the core of Bayesian decision theory (Robert 2007) and has attracted considerable attention in recent decades. Most approaches to the calculation of the required posterior model probabilities depend upon asymptotic arguments, the post-processing of outputs from Markov chain Monte Carlo (MCMC) algorithms operating on the space of a single model or using specially designed MCMC techniques that provide direct estimates of these quantities (e.g., reversible jump MCMC, RJMCMC; Green 1995). Within-model simulations are simpler, but generalizations of the harmonic mean estimator

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(Gelfand and Dey 1994) that are widely used in this setting require careful design to ensure finite variances and convergence assessment can be difficult. Simulations on the whole model space are often difficult to implement efficiently even though they can be conceptually appealing.

More robust and efficient Monte Carlo algorithms have been established in recent years. Many of them are population based, dealing with a collection of samples at each iteration, including sequential importance sampling and resampling (annealed importance sampling AIS, Neal 2001; sequential Monte Carlo SMC, Del Moral, Doucet, and Jasra 2006b) and population MCMC (PMCMC; Liang and Wong 2001; Jasra, Stephens, and Holmes 2007a). However, most studies have focused on their abilities to explore high-dimensional and multimodal spaces. The application of these algorithms to Bayesian model comparison is less well studied. Here, we motivate and present approaches based around the SMC family of algorithms, and demonstrate their effectiveness empirically.

SMC methods are a class of sampling algorithms, which combine importance sampling and resampling. They have been primarily used as “particle filters” to solve optimal filtering problems; see, for example, Cappé, Godsill, and Moulines (2007) and Doucet and Johansen (2011) for recent reviews. They are used here in a different manner, which were proposed by Del Moral, Doucet, and Jasra (2006b) and developed by Del Moral, Doucet, and Jasra (2006a) and Peters (2005). This framework employs a sequence of artificial distributions on spaces of increasing dimensions, which admit the distributions of interest as marginals.

Although it is well known that SMC is well suited to the computation of normalizing constants and that it is possible to develop relatively automatic SMC algorithms by employing a variety of “adaptive” strategies, their use for Bayesian model comparison has not yet received a great deal of attention. We highlight three strategies for computing posterior model probabilities using SMC, focusing on strategies that require minimal tuning and can be readily implemented requiring only the availability of *locally mixing* MCMC proposals. These methods admit natural and scalable parallelization and we demonstrate the potential of these algorithms with real implementations suitable for use on consumer-grade parallel computing hardware including GPUs, reinforcing the message of Lee et al. (2010). We also present a new approach to adaptation and guidelines on the near-automatic implementation of the proposed algorithms. These techniques are applicable to SMC algorithms in much greater generality. The proposed approach is compared with state-of-the-art alternatives in extensive simulation studies that demonstrate its performance and robustness.

The next section provides a brief survey of Bayesian model comparison literature. Section 3 presents three algorithms for performing model comparison using SMC techniques and Section 4 provides several illustrative applications, together with comparisons with other techniques. The article concludes with some discussion.

2. BACKGROUND

Bayesian model comparison depends upon the posterior distribution over models. It is only possible to obtain closed-form expressions for posterior model probabilities in very limited situations. The general problem has attracted considerable attention and it is not

feasible to exhaustively summarize this literature here. We describe the major contributions to the area and recent developments of particular relevance.

2.1 ANALYTIC METHODS AND MCMC

The Bayesian information criterion (BIC), developed by Schwarz (1978), is based upon a large sample approximation of the Bayes factor. An asymptotic argument concerning Bayes factors under appropriate regularity conditions justifies the choice of the model with the smallest value of BIC. Although appealing in its simplicity, justification requires the availability of a large number of observations.

The Bayesian approach to model comparison is, of course, to consider the posterior probabilities of the possible models (Bernardo and Smith 1994, chap. 6).

Given a denumerable collection of models $\{M_k\}_{k \in \mathcal{K}}$, with model M_k having parameter space Θ_k , Bayesian inference proceeds from a prior distribution over the collection of models, $\pi(M_k)$, a prior distribution for the parameters of each model, $\pi(\theta_k|M_k)$ and the (model-specific) likelihood $p(\mathbf{y}|\theta_k, M_k)$ to the model posterior:

$$\pi(M_k|\mathbf{y}) = \frac{p(\mathbf{y}|M_k)\pi(M_k)}{p(\mathbf{y})}, \quad (2.1)$$

where $p(\mathbf{y}|M_k) = \int_{\Theta_k} p(\mathbf{y}|\theta_k, M_k)\pi(\theta_k|M_k)d\theta_k$ is termed the *evidence* for model M_k and the normalizing constant $p(\mathbf{y}) = \sum_{k \in \mathcal{K}} p(\mathbf{y}|M_k)\pi(M_k)$ can be easily calculated if $|\mathcal{K}|$ is finite and the evidence for each model is available. The case where $|\mathcal{K}|$ is countable is discussed later. We first review some techniques for evidence calculation.

Several techniques have been proposed to approximate the evidence for a model using simulation techniques, which approximate the posterior distribution of that model, including the harmonic mean estimator of Newton and Raftery (1994), Raftery et al. (2006), and generalizations thereof (Gelfand and Dey 1994). These pseudo-harmonic mean methods use the insight that for any density g , such that $g(\cdot) \ll p(\cdot|\mathbf{y}, M_k)$, the following identity holds,

$$\int \frac{g(\theta_k)}{p(\mathbf{y}, \theta_k|M_k)} \pi(\theta_k|\mathbf{y}, M_k) d\theta_k = \int \frac{g(\theta_k)}{p(\mathbf{y}, \theta_k|M_k)} \frac{p(\mathbf{y}, \theta_k|M_k)}{p(\mathbf{y}|M_k)} d\theta_k = \frac{1}{p(\mathbf{y}|M_k)} \quad (2.2)$$

and by approximating the leftmost integral one can obtain an estimate of the evidence. Unfortunately, considerable care is required in the implementation of such schemes to control the variance of the resulting estimator—see Neal (1994).

In the particular case of the Gibbs sampler, Chib (1995) provided an alternative approach based on the identity,

$$p(\mathbf{y}|M_k) = \frac{p(\mathbf{y}|\theta_k, M_k)\pi(\theta_k|M_k)}{\pi(\theta_k|\mathbf{y}, M_k)}, \quad (2.3)$$

which holds for any value of θ_k . An estimator of the marginal likelihood can be obtained by replacing θ_k with a particular value, say θ_k^I , which is usually chosen from the high probability region of the posterior distribution and approximating the denominator $\pi(\theta_k^I|\mathbf{y}, M_k)$ using the output from a Gibbs sampler. Though this method does not suffer the instability associated with generalized harmonic mean estimators, it requires that all full conditional densities are known (including their normalizing constants) and that the Gibbs

sampler mixes adequately. This approach was generalized to other Metropolis–Hastings algorithms, by Chib and Jeliazkov (2001), who required only that the proposal distributions be known.

The RJMCMC strategy first proposed by Green (1995) is undoubtedly the most widespread approach that targets the joint posterior distribution over model and parameters. RJMCMC adapts the Metropolis–Hastings algorithm to construct a Markov chain on an extended state-space, which admits the posterior distribution over both model and parameters as its invariant distribution. The design of efficient between-model moves is often difficult, and the mixing of these moves largely determines the performance of the algorithm. For example, in multimodal models, where RJMCMC has attracted substantial attention, information available in the posterior distribution of a model of any given dimension does not characterize modes that exist only in models of higher dimension, and thus successful moves between those models become unlikely and difficult to construct (Jasra, Stephens, and Holmes 2007b). In addition, RJMCMC will not characterize models of low posterior probability well, as those models will be visited by the chain only rarely. In some cases, it will be difficult to determine whether the low acceptance rates of between-model moves result from actual characteristics of the posterior or from a poorly adapted proposal kernel.

A post-processing approach to improve the computation of normalizing constants from RJMCMC output using a bridge-sampling approach was advocated by Bartolucci, Scaccia, and Mira (2006). Sophisticated variants of these algorithms, such as those developed in Peters, Hayes, and Hossack (2010), have also been considered but depend upon essentially the same construction and ultimately require adequate mixing of the underlying Markov process.

Carlin and Chib (1995) presented an alternative method for simulating the model probability directly through a Gibbs sampler on the space $\{M_k\}_{k \in \mathcal{K}} \times \prod_{k \in \mathcal{K}} \Theta_k$. The joint parameter is thus (M, θ) where θ is the vector $(\theta_k)_{k \in \mathcal{K}}$ and conditional on model M_k the data \mathbf{y} only depend on a subset, θ_k , of the parameters. To form the Gibbs sampler, a so-called pseudoprior $\pi(\theta_k | M \neq M_k)$ in addition to the usual prior $\pi(\theta_k | M_k)$ is selected, such that given the model indicator M , the parameters associated with different models are conditionally mutually independent. In this way, a Gibbs sampler can be constructed provided that all the full conditional distributions $\pi(\theta_k | \mathbf{y}, \theta_{k' \neq k}, M)$ and $\pi(M = M_k | \mathbf{y}, \theta)$ for $k \in \mathcal{K}$ are available. The performance of this sampler, which was generalized by Godsill (2001), is very sensitive to the selected pseudopriors and sampling from the full conditional distribution must be feasible.

The methods reviewed above either demand substantial knowledge of the target distributions or require substantial tuning.

2.2 RECENT DEVELOPMENTS ON POPULATION-BASED METHODS

We consider two broad groups of population-based Monte Carlo methods. One family, including SMC, is based on sequential importance sampling and resampling. Another approach is population MCMC (PMCMC; Geyer 1991; Marinari and Parisi 1992; Liang and Wong 2001) also known as parallel tempering. PMCMC operates by constructing a sequence of distributions $\{\pi_t\}_{t=0}^T$ with π_0 corresponding to the target distribution and successive elements of this sequence consisting of distributions from which it is increasingly

easy to sample. A population of samples is maintained, with the i th element of the population being approximately distributed according to π_i ; the algorithm proceeds by simulating an ensemble of parallel MCMC chains each targeting one of these distributions. The chains interact with one another via exchange moves, in which the state of two adjacent chains is swapped, and this mechanism allows for information to be propagated between the chains and hopefully for the fast mixing of π_T to be partially transferred to the chain associated with π_0 . The resulting samples target the product $\prod_{t=0}^T \pi_t$, which admits π_0 as a marginal.

There is substantial interest in the use of population-based methods to explore high-dimensional and multimodal parameter spaces, which challenge conventional MCMC algorithms. Jasra, Stephens, and Holmes (2007a) compared the performance of the two approaches in this context. There is also increasing interest in using these methods for Bayesian model comparison. In principle, PMCMC output can be post-processed in the same way as conventional MCMC to obtain estimates of evidence for each model. However, this approach inherits many of the disadvantages of the basic estimators. Jasra, Stephens, and Holmes (2007b) combined PMCMC with RJMCMC and thus provided a direct estimate of the posterior model probability. Another approach is to use the outputs from all the chains to approximate the path sampling estimator (Gelman and Meng 1998), see Calderhead and Girolami (2009). However, the mixing speed of PMCMC is sensitive to the number and placement of the distributions $\{\pi_t\}_{t=0}^T$ (see Atchadé, Roberts, and Rosenthal (2010) for the optimal placement of distributions in terms of a particular mixing criterion for a restricted class of models). As seen in Calderhead and Girolami (2009), the placement of distributions can be critical—see Section 4.

The use of AIS for computing normalizing constants directly and via path sampling dates back at least to Neal (2001); see Vyshemirsky and Girolami (2008) for a recent example of its use in the computation of model evidences. It has often been suggested that more general SMC strategies provide no advantage over AIS when the normalizing constant is the object of inference. Later we will demonstrate that this is not generally true, adding improved robustness of normalizing constant estimates to the advantages afforded by resampling within SMC. This is consistent with theoretical results (Schweizer 2012) obtained in a slightly different context, which show that resampling can qualitatively improve the theoretical behavior of the estimator when the initial and final distributions differ substantially. More details on the use of SMC and path sampling for Bayesian model selection are provided in the next section. The use of PMCMC coupled with path sampling was discussed in Vyshemirsky and Girolami (2008).

Jasra et al. (2008) developed a method using a system of interacting SMC samplers for transdimensional simulation. The targeting distribution π and its space S are the same as in RJMCMC. As usual in SMC, a sequence of distributions $\{\tilde{\pi}_t\}_{t=0}^T$ with increasing dimensions are constructed such that $\tilde{\pi}_T$ admits π as a marginal. The algorithm starts with a set of SMC samplers with equal number of particles; each of them targets $\tilde{\pi}_{i,t}(x) \propto \tilde{\pi}_i(x)\mathbb{I}(x \in S_i)$ up to a predefined time index t^I , such that $\{S_i\}$ is a partition of S . At time t^I particles from all samplers are allowed to coalesce, and from this time on, all of them are iterated with the same Markov kernel (on S) until the single sampler reaches the target π . One of the three algorithms detailed in the next section coincides, essentially, with the final stage of the approach of Jasra et al. (2008); the other algorithms that are developed rely on a quite different strategy. We note that subsequent to the completion of the first version of this article, a related strategy has been proposed by Karagiannis and Andrieu (2013). They

combined SMC and MCMC via the mechanism of particle MCMC (Andrieu, Doucet, and Holenstein 2010) using an SMC algorithm as an RJMCMC proposal. This strategy is likely to lead to better mixing than conventional RJMCMC algorithm but comes at considerable computational cost.

A proof-of-concept study in which several SMC approaches to the problem were outlined was provided by Zhou, Johansen, and Aston (2012) and these approaches are developed below. These strategies based around various combinations of path sampling (Gelman and Meng 1998) and SMC (as used by Johansen, Del Moral, and Doucet (2006) in a rare events context and by Rousset and Stoltz (2006) in the context of the estimation of free energy differences) or the unbiased estimation of the normalizing constant via standard SMC techniques (Del Moral 1996; Del Moral, Doucet, and Jasra 2006b).

A strategy for SMC-based variable selection was developed by Schäfer and Chopin (2013); however, this approach depends upon the precise structure of this particular problem and does not involve the explicit computation of normalizing constants.

2.3 CHALLENGES FOR MODEL COMPARISON TECHNIQUES

There are a number of desirable features in algorithms that seek to address any model comparison problem and that these desiderata can find themselves in competition with one another. One always requires accurate evaluation of Bayes factors or model proportions and to obtain these one requires estimates of either normalizing constants or posterior model probabilities with small error making the efficiency of any Monte Carlo algorithm employed in their estimation critical. If one is interested in characterizing behavior conditional upon a given model or even calculating posterior-predictive quantities, it is likely to be necessary to explore the full parameter space of each model; this can be difficult if one employs between-model strategies that spend little time in models of low probability. In many settings, end-users seek to interpret the findings of model selection experiments and in such cases, accurate characterization of all models including those of relatively small probability may be important.

3. METHODOLOGY

SMC samplers provide, iteratively, collections of weighted samples from a sequence of distributions $\{\pi_t\}_{t=0}^T$ over essentially any random variables on some measurable spaces (E_t, \mathcal{E}_t) , by constructing a sequence of auxiliary distributions $\{\tilde{\pi}_t\}_{t=0}^T$ on spaces of increasing dimensions,

$$\tilde{\pi}_t(x_{0:t}) = \pi_t(x_t) \prod_{s=0}^{t-1} L_s(x_{s+1}, x_s), \quad (3.1)$$

where the sequence of Markov kernels $\{L_s\}_{s=0}^{t-1}$, termed backward kernels, is formally arbitrary but critically influences the estimator variance. See Del Moral, Doucet, and Jasra (2006b) for further details and guidance on the selection of these kernels.

Standard sequential importance resampling algorithms can then be applied to the sequence of synthetic distributions, $\{\tilde{\pi}_t\}_{t=0}^T$. At time $t = n - 1$, assume that a set of weighted particles $\{W_{n-1}^{(i)}, X_{0:n-1}^{(i)}\}_{i=1}^N$ approximating $\tilde{\pi}_{n-1}$ is available, then at time $t = n$, the path

of each particle is extended with a Markov kernel say, $K_n(x_{n-1}, x_n)$ yielding the set of particles $\{X_{0:n}^{(i)}\}_{i=1}^N$ and importance sampling is then applied. The weights are update by a factor \tilde{w}_n , termed the *incremental weights*, calculated as

$$\tilde{w}_n(x_{n-1}, x_n) = \frac{\pi_n(x_n)L_{n-1}(x_n, x_{n-1})}{\pi_{n-1}(x_{n-1})K_n(x_{n-1}, x_n)}. \quad (3.2)$$

If π_n is only known up to a normalizing constant, say $\pi_n(x_n) = \gamma_n(x_n)/Z_n$, then we can use the *unnormalized* incremental weights

$$w_n(x_{n-1}, x_n) = \frac{\gamma_n(x_n)L_{n-1}(x_n, x_{n-1})}{\gamma_{n-1}(x_{n-1})K_n(x_{n-1}, x_n)} \quad (3.3)$$

for importance sampling. Further, with the previously *normalized* weights $\{W_{n-1}^{(i)}\}_{i=1}^N$, we can estimate the ratio of normalizing constant Z_n/Z_{n-1} by

$$\frac{\hat{Z}_n}{Z_{n-1}} = \sum_{i=1}^N W_{n-1}^{(i)} w_n(X_{n-1:n}^{(i)}), \quad (3.4)$$

and

$$\frac{\hat{Z}_n}{Z_1} = \prod_{p=2}^n \frac{\hat{Z}_p}{Z_{p-1}} = \prod_{p=2}^n \sum_{i=1}^N W_{p-1}^{(i)} w_p(X_{p-1:p}^{(i)}) \quad (3.5)$$

provides an unbiased (Del Moral 2004, Proposition 7.4.1) estimate of Z_n/Z_1 . See Del Moral, Doucet, and Jasra (2006b) for details on calculating the incremental weights in general; in practice, when K_n is π_n -invariant, $\pi_n \ll \pi_{n-1}$, and L_{n-1} is the associated time-reversal kernel, the unnormalized incremental weight function becomes

$$w_n(x_{n-1}, x_n) = \frac{\gamma_n(x_{n-1})}{\gamma_{n-1}(x_{n-1})}. \quad (3.6)$$

This will be the situation throughout the remainder of this article.

3.1 SEQUENTIAL MONTE CARLO FOR MODEL COMPARISON

The problem of interest is characterizing the posterior distribution over $\{M_k\}_{k \in \mathcal{K}}$, a set of possible models, with model M_k having parameter vector $\theta_k \in \Theta_k$, which must also usually be inferred. Given prior distributions $\pi(M_k)$ and $\pi(\theta_k|M_k)$ and likelihood $p(y|\theta_k, M_k)$, we seek the posterior distributions $\pi(M_k|y) \propto p(y|M_k)$. There are three fundamentally different approaches to the computations:

1. Calculate posterior model probabilities directly.
2. Calculate the evidence, $p(y|M_k)$, of each model.
3. Calculate pairwise evidence ratios.

Each approach admits a natural SMC strategy. The relative strengths of these approaches and alternative methods are identified in Table 1.

Table 1. Strengths of algorithms for model choice. PMCMC admits a degree of parallelization, but is not a natural candidate for implementation on massively parallel architectures

	PHM	RJMCMC	PMCMC	SMC1	SMC2	SMC3
Can deal with a countable set of models		✓		✓		
Can exploit intermodel relationships		✓		✓		✓
Characterizes improbable models	✓		✓		✓	✓
Does not require reversible-pairs of moves	✓		✓	✓	✓	✓
Does not require intermodel mixing	✓		✓	✓	✓	
Admits straightforward parallelization			✓/×	✓	✓	✓
Does not rely upon ergodicity arguments				✓	✓	✓

3.1.1 SMC1: An All-in-One Approach. One could consider obtaining samples from the same distribution employed in the RJMCMC approach to model comparison, namely:

$$\pi^{(1)}(M_k, \theta_k) \propto \pi(M_k)\pi(\theta_k|M_k)p(\mathbf{y}|\theta_k, M_k), \quad (3.7)$$

which is defined on the disjoint union space $\bigcup_{k \in \mathcal{K}}(\{M_k\} \times \Theta_k)$.

One obvious SMC approach is to define a sequence of distributions $\{\pi_t^{(1)}\}_{t=0}^T$ such that $\pi_0^{(1)}$ is easy to sample from, $\pi_T^{(1)} = \pi^{(1)}$ and the intermediate distributions move smoothly between them. In the remainder of this section, we use the notation (M_t, θ_t) to denote a random sample on the space $\bigcup_{k \in \mathcal{K}}(\{M_k\} \times \Theta_k)$ at time t . One simple approach is the use of an annealing scheme such that

$$\pi_t^{(1)}(M_t, \theta_t) \propto \pi(M_t)\pi(\theta_t|M_t)p(\mathbf{y}|\theta_t, M_t)^{\alpha(t/T)}, \quad (3.8)$$

for some monotonically increasing $\alpha : [0, 1] \rightarrow [0, 1]$ such that $\alpha(0) = 0$ and $\alpha(1) = 1$. Other approaches are possible and might prove more efficient for some problems (such as the “data tempering” approach that Chopin (2002) proposed for parameter estimation—a strategy that would lend itself naturally to “online” estimation of evidence, but that would preclude the use of the path sampling estimator), but this strategy provides a convenient generic approach. These choices lead to Algorithm 1.

This approach might outperform RJMCMC when it is difficult to design fast-mixing Markov kernels. Such an SMC strategy can outperform MCMC at a given computational cost—see, for example, Fan, Leslie, and Wand (2008), Johansen, Doucet, and Davy (2008), and Fearnhead and Taylor (2010). Such transdimensional SMC has been proposed in several contexts (Peters 2005) and an extension proposed and analyzed by Jasra et al. (2008).

Algorithm 1 SMC1 : An All-in-One Approach to Model Comparison.

Initialization: Set $t \leftarrow 0$.

Sample $X_0^{(i)} = (M_0^{(i)}, \theta_0^{(i)}) \sim \nu$ for some proposal distribution ν (usually the joint prior).

Weight $W_0^{(i)} \propto w_0(X_0^{(i)}) = \pi(M_0^{(i)})\pi(\theta_0^{(i)}|M_0^{(i)})/\nu(M_0^{(i)}, \theta_0^{(i)})$.

Apply resampling if necessary (e.g., if ESS (Kong et al. 1994) less than some threshold).

Iteration: Set $t \leftarrow t + 1$.

Weight $W_t^{(i)} \propto W_{t-1}^{(i)}p(\mathbf{y}|\theta_t^{(i)}, M_{t-1}^{(i)})^{\alpha(t/T) - \alpha((t-1)/T)}$.

Apply resampling if necessary.

Sample $X_t^{(i)} \sim K_t(\cdot|X_{t-1}^{(i)})$, a $\pi_t^{(1)}$ -invariant kernel.

Repeat the Iteration step until $t = T$.

We include this approach for completeness and study it empirically later. Like other transdimensional methods, this approach depends upon collection of models being specified in advance. If new models are considered, then the entire simulation must be redone. The more direct approaches described in the following sections lead more naturally to easy-to-implement strategies with good performance.

3.1.2 SMC2: A Direct-Evidence-Calculation Approach. An alternative approach would be to estimate explicitly the evidence associated with each model. We propose to do this by sampling from a sequence of distributions for each model: starting from the parameter prior and sweeping through a sequence of distributions to the posterior.

Numerous strategies are possible to construct such a sequence of distributions, but one option is to use for each model M_k , $k \in \mathcal{K}$, the sequence $\{\pi_t^{(2,k)}\}_{t=0}^{T_k}$, defined by

$$\pi_t^{(2,k)}(\theta_t) \propto \pi(\theta_t | M_k) p(\mathbf{y} | \theta_t, M_k)^{\alpha_k(t/T_k)}, \quad (3.9)$$

where the number of distribution T_k , and the annealing schedule, $\alpha_k : [0, 1] \rightarrow [0, 1]$ may be different for each model. This leads to Algorithm 2.

The estimator of the posterior model probabilities depends upon the approach taken to estimate the normalizing constant. Direct estimation of the evidence can be performed using the output of this SMC algorithm and the standard estimator (Del Moral, Doucet, and Jasra 2006b, eq. (14)), termed SMC2-DS below:

$$\frac{1}{N} \sum_{i=1}^N \frac{\pi(\theta_0^{(k,i)} | M_k)}{v(\theta_0^{(k,i)})} \times \prod_{t=2}^T \sum_{i=1}^N W_{t-1}^{(k,i)} p(\mathbf{y} | \theta_{t-1}^{(k,i)} M_k)^{\alpha_k(t/T_k) - \alpha_k([t-1]/T_k)}, \quad (3.10)$$

where $W_{t-1}^{(k,i)}$ is the importance weight of sample i , $\theta_{t-1}^{(k,i)}$, *after* any resampling step of iteration $t-1$ for model M_k . This formula can be simplified by replacing $W_{t-1}^{(k,i)}$ with $1/N$ when resampling is conducted at every iteration (and it is unbiased); otherwise a mathematically simpler representation less naturally suited to computational use is provided by Del Moral, Doucet, and Jasra (2006b, eq. (15)). An alternative approach to computing the evidence is also worthy of consideration. As has been suggested, and shown empirically to perform well previously (see, e.g., Johansen, Del Moral, and Doucet 2006), it is possible to use all of the samples from every generation of an SMC sampler to approximate the path sampling estimator. Section 3.2 provides details.

The posterior distribution of the parameters conditional upon a particular model can also be approximated using

$$\hat{\pi}_{T_k}^{(2,k)}(d\theta) = \sum_{i=1}^N W_{T_k}^{(k,i)} \delta_{\theta_{T_k}^{(k,i)}}(d\theta).$$

This approach is appealing for several reasons. It is designed to estimate directly the quantity of interest: the evidence. It provides as good a characterization of each model as is required: it is possible to obtain a good estimate of the parameters of every model, even those for which the posterior probability is small (although, of course, in certain circumstances the automatic assignment of computational resources to the most promising models may be desirable). Perhaps most significant is that this approach does not require the design of proposal distributions or Markov kernels that move from one model to another:

each model is dealt with in isolation. While this may not be desirable in every situation, there are circumstances in which efficient moves between models are almost impossible to devise.

This approach also has some disadvantages. In particular, it is necessary to run a separate simulation for each model—rendering it impossible to deal with countable collections of models (although this is not such a substantial problem in many interesting cases). The ease of implementation may often offset this limitation.

Algorithm 2 SMC2 : A Direct-Evidence-Calculation Approach.

For each model $k \in \mathcal{K}$ execute the following algorithm.

Initialization: Set $t \leftarrow 0$.

Sample $\theta_0^{(k,i)} \sim \nu_k$ for some proposal distribution ν_k (usually the parameter prior).

Weight $W_0^{(k,i)} \propto w_0(\theta_0^{(k,i)}) = \pi(\theta_0^{(k,i)} | M_k) / \nu_k(\theta_0^{(k,i)})$.

Apply resampling if necessary.

Iteration: Set $t \leftarrow t + 1$.

Weight $W_t^{(k,i)} \propto W_{t-1}^{(k,i)} p(\mathbf{y} | \theta_{t-1}^{(k,i)}, M_k)^{\alpha(t/T_k) - \alpha((t-1)/T_k)}$.

Apply resampling if necessary.

Sample $\theta_t^{(k,i)} \sim K_t(\cdot | \theta_{t-1}^{(k,i)})$, a $\pi_t^{(k,2)}$ -invariant kernel.

Repeat the Iteration step until $t = T_k$.

3.1.3 SMC3: A Relative-Evidence-Calculation Approach. A final approach can be thought of as *sequential model comparison*. Rather than estimating the evidence associated with any particular model, we could estimate pairwise evidence ratios directly. The SMC sampler starts with an initial distribution being the posterior of one model (an initial sample could be obtained using a secondary SMC algorithm or other sampler) and moves toward the posterior of another related model. Then the sampler can continue toward another related model and so forth.

Given a finite collection of models $\{M_k\}$, $k \in \mathcal{K}$, suppose the models are ordered in a sensible way (e.g., M_{k-1} is nested within M_k or θ_k is of higher dimension than θ_{k-1}). For each $k \in \mathcal{K}$, we consider a sequence of distributions $\{\pi_t^{(3,k)}\}_{t=0}^{T_k}$, such that $\pi_0^{(3,k)}(M, \theta) = \pi(\theta | \mathbf{y}, M_k) \mathbb{I}_{\{M_k\}}(M)$ and $\pi_{T_k}^{(3,k)}(M, \theta) = \pi(\theta | \mathbf{y}, M_{k+1}) \mathbb{I}_{\{M_{k+1}\}}(M) = \pi_0^{(3,k+1)}(M, \theta)$. When it is possible to construct an SMC sampler that iterates over this sequence of distributions, the estimate of the ratio of normalizing constants is the Bayes factor estimate of model M_{k+1} in favor of model M_k .

This approach is conceptually appealing, but requires the construction of a smooth path between the posterior distributions of interest. The geometric annealing strategy that has been advocated as a good generic strategy in the previous sections is only appropriate when the support of successive distributions is nonincreasing. This is unlikely to be the case in interesting model comparison problems.

In this article, we consider a sequence of distributions on the disjoint union $\{M_k, \Theta_k\} \cup \{M_{k+1}, \Theta_{k+1}\}$, with the sequence of distributions $\{\pi_t^{(3,k)}\}_{t=0}^{T_k}$ defined as the full posterior,

$$\pi_t^{(3,k)}(M_t, \theta_t) \propto \pi_t(M_t) \pi(\theta_t | M_t) p(\mathbf{y} | \theta_t, M_t), \quad (3.11)$$

where $M_t \in \{M_k, M_{k+1}\}$ and the “prior” over models at time t , $\pi_t(M_{k+1}) := \alpha(t/T_k)$, for some monotonically increasing bijection $\alpha : [0, 1] \rightarrow [0, 1]$. The MCMC moves between need to be similar to those in the RJMCMC or SMC1 algorithms. However, instead of

efficient exploration of the whole model space, only moves between two models are required and the sequence of distributions employed helps to ensure exploration of both model spaces. Algorithm 3 uses this particular sequence of distribution but other sequence of distributions between models could be employed.

An advantage of this approach is that it provides direct estimates of the Bayes factor, which is of interest for model comparison purpose while not requiring exploration of as complicated a space as that employed within RJMCMC or SMC1. The estimation of normalizing constant in SMC3 follows in exactly the same manner as in the SMC2 case. In SMC3, the same estimator provides a direct estimate of the Bayes factor.

Algorithm 3 SMC3: A Relative-Evidence-Calculation Approach to Model Comparison.

Initialization: Set $k \leftarrow 1$.

Use Algorithm 2 to obtain weighted samples for $\pi_{T_1}^{(3,1)}$, the parameter posterior for model M_1

Relative Evidence Calculation

Set $k \leftarrow k + 1$, $t \leftarrow 0$.

Denote current weighted samples as $\{W_0^{(k,i)}, X_0^{(k,i)}\}_{i=1}^N$, where $X_0^{(k,i)} = (M_0^{(k,i)}, \theta_0^{(k,i)})$

Apply resampling if necessary.

Iteration: Set $t \leftarrow t + 1$.

Weight $W_t^{(k,i)} \propto W_{t-1}^{(k,i)} \pi_t(M_{t-1}^{(k,i)}) / \pi_{t-1}(M_{t-1}^{(k,i)})$.

Apply resampling if necessary.

Sample $(M_t^{(k,i)}, \theta_t^{(k,i)}) \sim K_t(\cdot | M_{t-1}^{(k,i)} \theta_{t-1}^{(k,i)})$, a $\pi_t^{(3,k)}$ -invariant kernel.

Repeat the Iteration step up to $t = T_k$.

Repeat the Relative Evidence Calculation step until sequentially all relative evidences are calculated.

3.2 PATH SAMPLING VIA SMC2/SMC3

A Monte Carlo approximation of the *path sampling* identity (Gelman and Meng 1998) (also known as thermodynamic integration or Ogata's method) also provides an estimate of the normalizing constant. The use of AIS for the same purpose (Neal 2001) is common in some settings; as will be demonstrated below the incorporation of some other elements of the more general SMC algorithm family can improve performance at negligible cost. Given a parameter α that defines a family of distributions, $\{p_\alpha = q_\alpha / Z_\alpha\}_{\alpha \in [0,1]}$ that move smoothly from $p_0 = q_0 / Z_0$ to $p_1 = q_1 / Z_1$ as α increases from zero to one. The logarithm of the ratio of their normalizing constants satisfies a simple integral relationship under mild regularity conditions:

$$\log\left(\frac{Z_1}{Z_0}\right) = \int_0^1 \mathbb{E}_\alpha \left[\frac{d \log q_\alpha(\cdot)}{d\alpha} \right] d\alpha, \quad (3.12)$$

where \mathbb{E}_α denotes expectation under p_α ; see Gelman and Meng (1998). Note that the sequence of distributions in the SMC2 and SMC3 algorithms above, can both be interpreted as belonging to such a family of distributions, with $\alpha_t = \alpha(t/T_k)$, where the mapping $\alpha : [0, 1] \rightarrow [0, 1]$ is again monotonic with $\alpha(0) = 0$ and $\alpha(1) = 1$.

The SMC sampler provides us with a set of weighted samples obtained from a sequence of distributions suitable for approximating this integral. At each t , we can obtain an estimate of the expectation within the integral for $\alpha(t/T)$ via the usual importance sampling

estimator, and this integral can then be approximated via numerical integration. Whenever the sequence of distributions employed by SMC3 has appropriate differentiability, it is also possible to employ path sampling to estimate, directly, the evidence ratio via this approach applied to the samples generated by that algorithm. In general, given an increasing sequence $\{\alpha_t\}_{t=0}^T$ where $\alpha_0 = 0$ and $\alpha_T = 1$, a family of distributions $\{p_\alpha\}_{\alpha \in [0,1]}$ as before, and an SMC sampler that iterates over the sequence of distribution $\{\pi_t = p_{\alpha_t} = q_{\alpha_t}/Z_{\alpha_t}\}_{t=0}^T$, then with the weighted samples $\{W_t^{(j)}, X_t^{(j)}\}_{j=1}^N$, and $t = 0, \dots, T$, a path sampling estimator of the ratio of normalizing constants $\Xi_T = \log(Z_1/Z_0)$ can be approximated (using an elementary trapezoidal scheme) by

$$\widehat{\Xi}_T^N = \sum_{t=1}^T \frac{1}{2}(\alpha_t - \alpha_{t-1})(U_t^N + U_{t-1}^N), \quad (3.13)$$

where

$$U_t^N = \sum_{j=1}^N W_t^{(j)} \frac{d \log q_\alpha(X_t^{(j)})}{d\alpha} \Big|_{\alpha=\alpha_t}. \quad (3.14)$$

We term these estimators SMC2-PS and SMC3-PS. The combination of SMC and path sampling is somewhat natural and has been proposed before, for example, Johansen, Del Moral, and Doucet (2006) although not there in a Bayesian context. The estimation of normalizing constants by this approach seems to have received little attention in the literature. Perhaps because of widespread acceptance of the suggestion of Del Moral, Doucet, and Jasra (2006b) that SMC does not outperform AIS when normalizing constants are the object of inference or that of Calderhead and Girolami (2009) that all simulation-based estimators based around path sampling can be expected to behave similarly. We will demonstrate below that these observations, while true in certain contexts, do not hold in full generality.

3.3 EXTENSIONS AND REFINEMENTS

3.3.1 Improved Univariate Numerical Integration. The path sampling estimator requires evaluation of the expectation, $\mathbb{E}_\alpha[d \log q_\alpha/d\alpha]$ for $\alpha \in [0, 1]$, which can be approximated by importance sampling using samples generated by an SMC sampler operating on the sequence of distributions $\{\pi_t = p_{\alpha_t} = q_{\alpha_t}/Z_{\alpha_t}\}_{t=0}^T$ directly for $\alpha \in \{\alpha_t\}_{t=0}^T$. For any $\alpha \in [0, 1]$, by finding t such that $\alpha \in (\alpha_{t-1}, \alpha_t)$, the expectation can be approximated using existing SMC samples—the quantities required to obtain such an estimate have already been calculated during the running of the SMC algorithm and such computations have little computational cost.

As noted by Friel, Hurn, and Wyse (2014), we can use more sophisticated numerical integration strategies to reduce the path sampling estimator bias. In the case of SMC, it is especially straightforward to estimate the required expectations at arbitrary α and so higher order integration can be used cheaply. Numerical integrations that make use of a finer mesh $\{\alpha'_t\}_{t=0}^{T'}$ than $\{\alpha_t\}_{t=0}^T$ can be easily implemented. Due to the possible instability of numerical integrations based on approximations of derivatives, the second approach can

be more appealing in some applications. A demonstration of the bias reduction effect is provided in Section 4.2.

3.3.2 Adaptive Specification of Distributions. As the importance weights at time t depend only upon the sample at time $t - 1$, it is relatively straightforward to consider sample-dependent, adaptive specification of the sequence of distributions (typically by choosing the value of a parameter, such as $\alpha_t = \alpha(t/T_k)$ in the settings of SMC2 and SMC3, based upon the current sample). Jasra et al. (2010) proposed such a method based on controlling the rate at which the effective sample size (ESS; Kong, Liu, and Wong 1994) falls. With little computation cost, this provides an automatic method of specifying a tempering schedule in such a way that the ESS decays in a regular fashion. Schäfer and Chopin (2013, Algorithm 2) used a similar technique but by moving the particle system only when it resamples they are in a setting equivalent to resampling at every timestep (with longer time steps, followed by multiple applications of the MCMC kernel) in our formulation. We advocate resampling adaptively only when the ESS is smaller than a preset threshold, and here we propose a more general adaptive scheme for the selection of the sequence of distributions that has better properties when adaptive resampling is employed.

The ESS was designed to assess the loss of efficiency arising from the use of a simple weighted sample (rather than a simple random sample from the distribution of interest) in the computation of expectations. It is obtained by considering a sample approximation of a low-order Taylor expansion of the variance of the importance sampling estimator of an arbitrary test function to that of the simple Monte Carlo estimator; the test function vanishes from the expression as a consequence of this expansion.

In our context, allowing $W_{t-1}^{(i)}$ to denote the *normalized weights* of particle i at the end of time $t - 1$, and $w_t^{(i)}$ to denote the *unnormalized* incremental weights of particle i during iteration t , the ESS calculated using the current weight of each particle is simply

$$\text{ESS}_t = \left[\sum_{j=1}^N \left(\frac{W_{t-1}^{(j)} w_t^{(j)}}{\sum_{k=1}^N W_{t-1}^{(k)} w_t^{(k)}} \right)^2 \right]^{-1} = \frac{(\sum_{j=1}^N W_{t-1}^{(j)} w_t^{(j)})^2}{\sum_{k=1}^N (W_{t-1}^{(k)})^2 (w_t^{(k)})^2}. \quad (3.15)$$

It is clearly appropriate to use this quantity (which corresponds to the coefficient of variation of the current normalized importance weights) to assess weight degeneracy and to make decisions about appropriate resampling times (see Del Moral, Doucet, and Jasra 2012) but it is rather less apparent that it is the correct quantity to consider when adaptively specifying a sequence of distributions in an SMC sampler.

The ESS of the current sample weights tells us about the accumulated mismatch between proposal and target distributions (on an extended space including the full trajectory of the sample paths) since the last resampling time. Fixing either the relative or absolute reduction in ESS between successive distributions does *not* lead to a common discrepancy between successive distributions unless resampling is conducted after every iteration as will be demonstrated below.

When specifying a sequence of distributions it is natural to aim for a similar discrepancy between each pair of successive distributions. The natural question to ask is consequently, how large can we make $\alpha_t - \alpha_{t-1}$ while ensuring that π_t remains sufficiently similar to π_{t-1} . One way to measure the discrepancy would be to consider how good an importance

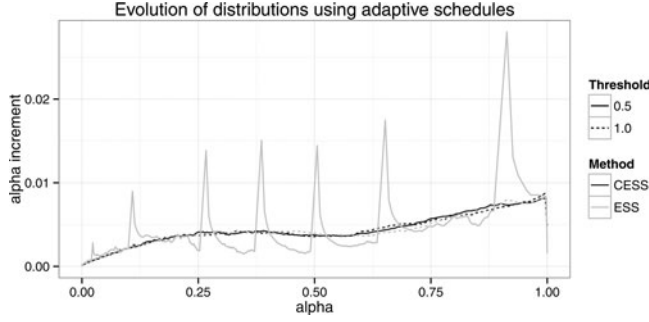


Figure 1. A typical plot of $\alpha_t - \alpha_{t-1}$ against α_t (for a Gaussian mixture model example using the SMC2 algorithm; see the supplementary material). All four samplers use roughly the same number of distributions.

sampling proposal π_{t-1} would be for the estimation of expectations under π_t and a natural way to measure this is via the sample approximation of a Taylor expansion of the relative variance of such an estimator exactly as in the ESS .

Such a procedure (see the supplementary material for its derivation) leads us to a quantity that we have termed the *conditional* ESS (CESS):

$$\text{CESS}_t = \left[\sum_{j=1}^N N W_{t-1}^{(j)} \left(\frac{w_t^{(j)}}{\sum_{k=1}^N N W_{t-1}^{(k)} w_t^{(k)}} \right)^2 \right]^{-1} = \frac{N (\sum_{j=1}^N W_{t-1}^{(j)} w_t^{(j)})^2}{\sum_{k=1}^N W_{t-1}^{(k)} (w_t^{(k)})^2}, \quad (3.16)$$

which is equal to the ESS only when resampling is conducted during every iteration. The bracketed term coincides with a sample approximation (using the actual sample that is properly weighted to target π_{t-1}) of the expected sum of the unnormalized weights squared divided by the square of a sample approximation of the expected sum of unnormalized weights when considering sampling from π_{t-1} and targeting π_t by simple importance sampling.

Figure 1 shows the variation of $\alpha_t - \alpha_{t-1}$ with α_t when fixed reductions in ESS and CESS are used to specify the sequence of distributions both when resampling is conducted during every iteration (or equivalently, when the ESS/ N falls below a threshold of 1.0) and when resampling is conducted only when the ESS/ N falls below a threshold of 0.5. As is demonstrated in Section 4 the CESS-based scheme leads to a reduction in estimator variance of around 20% relative to a manually tuned (quadratic; see the supplementary material) schedule while the ESS-based strategy provides little improvement over the linear case unless resampling is conducted during every iteration.

In addition to providing a significantly better performance at essentially no cost, the use of the CESS emphasizes the purpose of the adaptive specification of the sequence of distributions: to produce a sequence in which the difference between each successive pair is the same (when using the CESS one is seeking to ensure that the variance of the importance weights one would arrive at if using π_{t-1} as a proposal for π_t is constant).

We note that the standard estimate of the normalizing constant need not be unbiased when adaptive techniques are employed. However, a very recent analysis (Beskos, Jasra, and Thiéry 2013) provides some formal justification of the use of both adaptive tempering schedules and adaptive specification of proposals, the topic of the next section.

3.3.3 Adaptive Specification of Proposals. The SMC sampler is remarkably robust to the mixing speed of MCMC kernels employed (see the empirical study below). However, as with any sampling algorithms, faster mixing does not harm performance and in some cases will considerably improve it. For random walk Metropolis kernels, the mixing speed depends upon the proposal *scale*.

We adopt an approach similar to Jasra et al. (2010) who used sample covariance estimates to inform the proposal covariance for the next iteration. We found that such an approach generally produces satisfactory results and it is simple to implement. In difficult problems alternative approaches could be employed; one approach demonstrated by Jasra et al. (2010) is to simply employ a pair of acceptance rate thresholds and to alter the proposal scale from the simply estimated value whenever the acceptance rate falls outside those threshold values. Beskos, Jasra, and Thiéry (2013) showed, convergence results for this kind of adaptive specification of Markov kernels.

More sophisticated proposal strategies could undoubtedly improve performance further and their use warrants investigation. One appealing approach is using the Metropolis adjusted Langevin algorithm (MALA; see Roberts and Tweedie 1996). We could use the particle approximation at time index $t = n - 1$ to estimate the covariance matrix of π_n and thus tune the scale h online. As these algorithms are known to be somewhat sensitive to scaling, and we seek approaches robust enough to employ with little user intervention, we have not investigated this strategy here.

3.4 A NEAR-AUTOMATIC, GENERIC ALGORITHM

With the above refinements, the SMC2 algorithm can be implemented with minimal tuning and application-specific effort while providing robust and accurate estimates of the model evidence $p(\mathbf{y}|M_k)$. The geometric annealing path that connects the prior $\pi(\theta_k|M_k)$ and the posterior $\pi(\theta_k|\mathbf{y}, M_k)$ provides a smooth path for a wide range of problems. The actual annealing schedule under this scheme can be determined using the adaptive schedule as described above. Finally, we can adaptively specify the Metropolis random walk (or MALA) scales through the estimation of their scaling parameters as the sampler iterates. In contrast to the MCMC setting, where such adaptive algorithms will usually require a burn-in period, which will not be used for further estimation, in SMC, the variance and covariance estimates come at almost no cost, as all the samples will later be used for marginal likelihood estimation. Additionally, adaptation within SMC does not require separate theoretical justification—something that can significantly complicate the development of adaptive schemes in the MCMC setting. We outline the adaptive form of SMC2 in Algorithm 4.

As laid out above, the algorithm requires minimal tuning. Its robustness, accuracy, and efficiency will be shown empirically in Section 4. Automating SMC1 is less straightforward as the between model moves still require effort to design and implement. In SMC3, the specification of the sequences between posterior distributions are less generic than the geometric annealing scheme in SMC2. However, the adaptive schedule and automatic tuning of MCMC proposal scales can readily be applied.

Some auxiliary inputs are still required. However, for a given class of models, with minimal tuning, the algorithm can be carried out in a nearly automatic fashion for different

Algorithm 4 An Automatic, Generic Algorithm for Bayesian Model Comparison.

Accuracy control

Set constant $\text{CESS}^I \in (0, 1)$, using a small pilot simulation if necessary.

Initialization: Set $t \leftarrow 0$.

Perform the *Initialization* step as in Algorithm 2

Iteration: Set $t \leftarrow t + 1$

Step size selection

Use a binary search to find α^I such that $\text{CESS}_{\alpha^I} = \text{CESS}^I$

Set $\alpha_t \leftarrow \alpha^I$ if $\alpha^I \leq 1$, otherwise set $\alpha_t \leftarrow 1$

Proposal scale calibration

Computing the importance sampling estimates of first two moments of parameters.

Set the proposal scale of the Markov proposal K_t with the estimated parameter variances.

Perform the *Iteration* step as in Algorithm 2 with the found α_t and proposal scales.

Repeat the Iteration step until $\alpha_t = 1$ then set $T = t$.

data or model settings, in the sense that these inputs do not need to be done on a per model or per dataset basis. We believe this framework presented here is at least a good foundation for building automatic model comparison procedures for many application areas.

Although further enhancements and refinements are clearly possible, we focus in the remainder of this article on this simple, generic algorithm that can be easily implemented in any application and has proved sufficiently powerful to provide good estimation in the examples we have encountered thus far.

4. ILLUSTRATIVE APPLICATIONS

A classical Gaussian mixture model (GMM) as formulated in Del Moral, Doucet, and Jasra (2006b) was first used to compare all three SMC algorithms with RJMCMC, AIS, and PMCMC. The details of model setting and results are in the supplementary material. It was found that all five algorithms agree on the results while the performance in terms of Monte Carlo variance varies considerably. We reached the conclusion that the SMC2 algorithm with adaptive strategies is the most promising among the SMC strategies, considering ease of implementation, performance, and generality. Also, while it has been suggested that AIS might perform similarly to SMC for the estimation of normalizing constants, the GMM example shows that resampling can have a beneficial effect on the variance allowing SMC to outperform AIS in practice.

In this section, two realistic examples, a nonlinear ordinary differential equation (ODE) model and a positron emission tomography compartmental model are used to study the performance and robustness of algorithm SMC2 compared to AIS and PMCMC. Various configurations of the algorithms are considered including both sequential and parallelized implementations.

The C++ implementations, which make use of the vSMC library of Zhou (2013), of all examples can be found at <https://github.com/zhouyan/vSMC>.

4.1 NONLINEAR ORDINARY DIFFERENTIAL EQUATIONS

In this section, SMC2 will now be further explored in a more complex model, a nonlinear ordinary differential equations system. This model, which was studied by Calderhead and

Girolami (2009), is known as the Goodwin model. The ODE system, for an m -component model, is

$$\begin{aligned}\frac{dX_1(t)}{dt} &= \frac{a_1}{1 + a_2 X_m(t)^\rho} - \alpha X_1(t) \\ \frac{dX_i(t)}{dt} &= k_{i-1} X_{i-1}(t) - \alpha X_i(t) \quad i = 2, \dots, m \\ X_i(0) &= 0 \quad i = 1, \dots, m.\end{aligned}$$

The parameters $\{\alpha, a_1, a_2, k_{1,m-1}\}$ have common prior distribution $\mathcal{G}(0.1, 0.1)$. Under this setting, $X_{1:m}(t)$ can exhibit either unstable oscillation or a constant steady state. The data are simulated for $m = \{3, 5\}$ at equally spaced time points from 0 to 60, with time step 0.5. The last 80 data points of $(X_1(t), X_2(t))$ are used for inference. Normally distributed noise with standard deviation $\sigma = 0.2$ is added to the simulated data. Following Calderhead and Girolami (2009), the variance of the additive measurement error is assumed to be known. Therefore, the posterior distribution has $m + 2$ parameters for an m -component model.

As shown by Calderhead and Girolami (2009), when $\rho > 8$, due to the possible instability of the ODE system, the posterior can have a considerable number of local modes. In this example, we set $\rho = 10$. Also, as the solution to the ODE system is somewhat unstable, slightly different data can result in very different posterior distributions.

4.1.1 Results. We compare results from the SMC2 and PMCMC algorithms. For the SMC implementation, 1000 particles and 500 iterations were used, with the distributions specified by Equation (3.9), with $\alpha(t/T) = (t/T)^5$, or via the completely adaptive specification. For the PMCMC algorithm, 50,000 iterations are performed for burn-in and another 10,000 iterations are used for inference. The same tempering as was used for SMC is used here. Note that, in a sequential implementation of PMCMC, with each iteration updating one local chain and attempting a global exchange, the computational cost of after burn-in iterations is roughly the same as the entire SMC algorithm. In addition, changing T within the range of the number of cores available does not substantially change the computational cost of a generic parallel implementation of the PMCMC algorithm, with each iteration updating all local chains concurrently. We compare results from $T = 10, 30, 100$ for PMCMC and $T = 500$ (or close to this number when the distributions are specified adaptively) for SMC. The results for data generated from the simple model ($m = 3$) and complex model ($m = 5$), summarizing variability among 100 runs of each algorithm, are shown in Tables 2 and 3, respectively.

As shown in both cases, the number of distributions can affect the performance of PMCMC algorithms considerably. When using 10 distributions, large bias from numerical integration for path sampling estimator was observed, as expected. With 30 distributions, the performance is comparable to the SMC2 sampler, though some bias is still observable. With 100 distributions, there is a much larger variance because, with more chains, the information travels more slowly from rapidly mixing chains to slowly mixing ones and consequently the mixing of the overall system is inhibited.

The SMC algorithm provides results comparable to the best of three PMCMC implementations in all settings, including one in which both the annealing schedule and proposal

Table 2. Results for nonlinear ODE models with data generated from simple model. *Italic*: Minimum variance for particular algorithm. **Bold**: Minimum variance among samplers

T	Proposal scales	Annealing scheme	Algorithm	Marginal likelihood ($\log p(\mathbf{y} M_k) \pm \text{SD}$)		Bayes factor $\log B_{3,5}$
				$m = 3$	$m = 5$	
10	Manual	Prior (5)	PMCMC	-109.7 ± 3.2	-120.3 ± 2.5	10.6 ± 3.8
30				-105.0 ± 1.2	-116.1 ± 2.2	11.2 ± 2.5
100				-134.7 ± 7.9	-144.1 ± 6.2	9.4 ± 11.2
500	Manual	Prior (5)	SMC2-DS	-104.6 ± 2.0	-112.7 ± 1.8	8.1 ± 2.8
			SMC2-PS	-104.5 ± 1.8	-112.7 ± 1.5	8.2 ± 2.5
500	Manual	Adaptive	SMC2-DS	-104.5 ± 1.1	-112.7 ± 1.1	8.1 ± 1.6
			SMC2-PS	-104.6 ± 1.0	-112.8 ± 1.0	8.2 ± 1.5
500	Adaptive	Adaptive	SMC2-DS	-104.5 ± 0.5	-112.7 ± 0.4	8.1 ± 0.8
			SMC2-PS	-104.6 ± 0.4	-112.8 ± 0.3	8.1 ± 0.6

scaling were fully automatic, and significantly better for the data generated from simple model. In fact, the completely adaptive strategy was the most successful.

It can be seen that in contrast to the PMCMC algorithm, the SMC algorithm can increase the number of the distributions to reduce the bias of the numerical integration for the path sampling estimator without increasing the Monte Carlo variance.

4.2 POSITRON EMISSION TOMOGRAPHY COMPARTMENTAL MODEL

It is now interesting to compare the proposed algorithm with other state-of-art algorithms using a realistic example.

Positron emission tomography (PET) is a technique used for studying the brain in vivo, most typically when investigating metabolism or neuro-chemical concentrations in either normal or patient groups. Given the nature and number of observations typically recorded in time, PET data are usually modeled with linear differential equation systems. For an overview of PET compartmental models, see Gunn et al. (2002). Given data $(y_1, \dots, y_n)^T$,

Table 3. Results for nonlinear ODE models with data generated from complex model. *Italic*: Minimum variance for particular algorithm. **Bold**: Minimum variance among samplers

T	Proposal scales	Annealing scheme	Algorithm	Marginal likelihood ($\log p(\mathbf{y} M_k) \pm \text{SD}$)		Bayes factor $\log B_{5,3}$
				$m = 3$	$m = 5$	
10	Manual	Prior (5)	PMCMC	-1651 ± 27.9	-85.1 ± 36.6	1566 ± 42.1
30				-1640 ± 7.4	-78.9 ± 11.2	1561 ± 12.8
100				-1625 ± 15.7	-75.7 ± 24.8	1549 ± 25.6
500	Manual	Prior (5)	SMC2-DS	-1641 ± 10.8	-78.5 ± 9.8	1562 ± 10.1
			SMC2-PS	-1641 ± 8.4	-79.2 ± 7.9	1562 ± 8.5
500	Manual	Adaptive	SMC2-DS	-1640 ± 6.9	-78.6 ± 4.8	1561 ± 7.1
			SMC2-PS	-1640 ± 5.4	-78.8 ± 3.7	1561 ± 6.8
500	Adaptive	Adaptive	SMC2-DS	-1640 ± 2.2	-79.4 ± 1.7	1560 ± 3.1
			SMC2-PS	-1640 ± 1.9	-78.5 ± 1.5	1562 ± 2.3

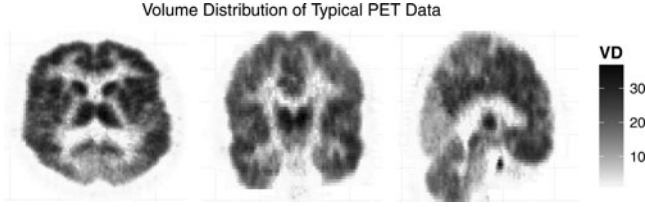


Figure 2. Estimates of V_D from a single PET scan as found using SMC2. The data show that the volume of distribution exhibits substantial spatial variation. Note that each pixel in the image represents an estimate from an individual time series. There are approximately 250,000 of them and each requires a Monte Carlo simulation to select a model.

an m -compartmental model has generative form:

$$y_j = C_T(t_j; \phi_{1:m}, \theta_{1:m}) + \sqrt{\frac{C_T(t_j; \phi_{1:m}, \theta_{1:m})}{t_j - t_{j-1}}} \varepsilon_j \quad (4.1)$$

$$C_T(t_j; \phi_{1:m}, \theta_{1:m}) = \sum_{i=1}^m \phi_i \int_0^{t_j} C_P(s) e^{-\theta_i(t_j-s)} ds, \quad (4.2)$$

where t_j is the measurement time of y_j , ε_j is additive measurement error and input function C_P is (treated as) known. The parameters $\phi_1, \theta_1, \dots, \phi_m, \theta_m$ characterize the model dynamics. See Zhou, Aston, and Johansen (2013) for applications of Bayesian model comparison for this class of models and details of the specification of the measurement error. In the simulation results below, ε_j are independently and identically distributed according to a zero mean Normal distribution of unknown variance, σ^2 , which was included in the vector of model parameters.

Real neuroscience datasets involve a very large number of time series ($\sim 200,000$ per brain), which are typically somewhat heterogenous. Figure 2 shows estimates of $V_D = \sum_{j=1}^m \phi_j / \theta_j$ from a typical PET scan (generated using SMC2 as will be discussed later). Robustness is therefore especially important. An application-specific MCMC algorithm was developed for this problem in Zhou, Aston, and Johansen (2013). A significant amount of tuning of the algorithms was required to obtain good results. The results shown in Figure 2 are very close to those of Zhou, Aston, and Johansen (2013) but, as is shown later, they were obtained with almost no manual tuning effort and at similar computational cost.

For SMC and PMCMC algorithms, the requirement of robustness means that the algorithm must be able to calibrate itself automatically to different data (and thus different posterior surfaces). A sequence of distributions that performs well for one time series may not perform even adequately for another series. Specification of proposal scales that produces fast-mixing kernels for one data series may lead to slow mixing for another. In the following experiment, we will use a single simulated time series, and choose schedules that performs both well and poorly for this particular time series. The objective is to see if the algorithm can recover from a relatively poorly specified schedule and obtain reasonably accurate results.

4.2.1 Results. In this example, we focus on the comparison between SMC2 and PMCMC. We also consider parallelized implementations of algorithms. In this case, due to

its relatively small number of chains, PMCMC can be parallelized completely (and often cannot fully use the hardware capability if a naïve approach to parallelization is taken; while we appreciate that more sophisticated parallelization strategies are possible, these depend intrinsically upon the model under investigation and the hardware employed and given our focus on automatic and general algorithms, we do not consider such strategies here). The PMCMC algorithm under this setting is implemented such that each chain is updated at each iteration. Further, for the SMC algorithms, we consider two cases. In the first, we can parallelize the algorithm completely (in the sense that each core has a single particle associated with it). In this setting, we use a relatively small number of particles and a larger number of time steps. In the second, we need a few passes to process a large number of particles at each time step, and accordingly we use fewer time steps to maintain the same total computation time. These two settings allow us to investigate the trade-off between the number of particles and time steps. In both implementations, we consider three schedules, $\alpha(t/T) = t/T$ (linear), $\alpha(t/T) = (t/T)^5$ (prior), and $\alpha(t/T) = 1 - (1 - t/T)^5$ (posterior). In addition, the adaptive schedule based upon CESS is also implemented for the SMC2 algorithm.

Results from 100 replicate runs of the two algorithms under various regimes can be found in Tables 4 and 5 for the marginal likelihood and Bayes factor estimates, respectively. The SMC algorithms consistently outperforms the PMCMC algorithms in the parallel settings. The Monte Carlo SD of SMC algorithms is typically of the order of one-fifth of the corresponding estimates from PMCMC in most scenarios. In some settings with the smaller number of samples, the two algorithms can be comparable. Also at the lowest computational costs, the samplers with more time steps and fewer particles outperform those with the converse configuration by a fairly large margin in terms of estimator variance. It shows that with limited resources, ensuring the similarity of consecutive distributions, and thus good mixing, can be more beneficial than a larger number of particles. However, when the computational budget is increased, the difference becomes negligible. The robustness of SMC to the change of schedules is again apparent.

It can also be seen that increasing the number of distributions not only reduces the path sampling estimator bias (as seen in the previous example), but also reduces the variances considerably given the same number of particles. On the other hand, increasing the number particles can only reduce the variance of the estimates, in accordance with the central limit theorem; see Del Moral, Doucet, and Jasra (2006b) for the standard estimator and extensions for the path sampling estimator, Proposition 1 in the supplementary material. (As the bias arises from numerical integration approximation of the path sampling estimator.)

Effects of Adaptive Schedule. A set of samplers with adaptive schedules are also used. Due to the nature of the schedule, it cannot be controlled to have exactly the same number of time steps as nonadaptive procedures. However, the CESS was controlled such that the average number of time steps are comparable with the fixed schedules and in most cases slightly less than the fixed numbers.

It is found that, with little computational overhead, adaptive schedules do provide the best results (or very nearly so) and do so without user intervention. The reduction of Monte Carlo SD varies among different configurations. For moderate or larger number of distributions, a reduction about 50% was observed. In addition, it shall be noted that, in this

Table 4. Marginal likelihood estimates of two component PET model. T : Number of distributions in SMC and number of iterations used for inference in PMCMC. N : Number of particles in SMC and number chains in PMCMC. The PMCMC and SMC with $N = 192$ are completely N -way parallelized. SMC with $N = 960$ are $N/5$ -way parallelized. *Italic*: Minimum variance for the same computational cost and the same proposal scales and annealing schemes. **Bold**: Minimum variance for the same computational cost and all proposal scales and annealing schemes

Proposal scales			Manual			Adaptive
Annealing scheme			Prior (5)	Posterior (5)	Adaptive	
T	N	Algorithm	Marginal likelihood estimates ($\log p(y M_k) \pm \text{SD}$)			
500	30	PMCMC	-39.1 ± 0.56	-926.8 ± 376.99		
500	192	SMC2-DS	-39.2 ± 0.25	-39.7 ± 1.06	-39.2 ± 0.18	-39.1 ± 0.12
		SMC2-PS	-39.2 ± 0.25	-91.3 ± 21.69	-39.2 ± 0.18	-39.1 ± 0.13
100	960	SMC2-DS	-39.3 ± 0.36	-40.6 ± 1.41	-39.2 ± 0.31	-39.2 ± 0.19
		SMC2-PS	-39.3 ± 0.35	302.1 ± 46.29	-39.3 ± 0.31	-39.2 ± 0.18
5000	30	PMCMC	-39.3 ± 0.21	-917.6 ± 129.54		
5000	192	SMC2-DS	-39.2 ± 0.09	-39.2 ± 0.20	-39.2 ± 0.08	-39.1 ± 0.04
		SMC2-PS	-39.2 ± 0.09	-43.8 ± 2.13	-39.2 ± 0.08	-39.1 ± 0.04
1000	960	SMC2-DS	-39.2 ± 0.08	-39.2 ± 0.31	-39.2 ± 0.07	-39.2 ± 0.03
		SMC2-PS	-39.2 ± 0.08	-65.7 ± 5.54	-39.2 ± 0.07	-39.2 ± 0.03

example, the bias of path sampling estimates are much more sensitive to the schedules than the previous Gaussian mixture model example. A vanilla linear schedule does not provide a low bias estimator at all even when the number of distributions is increased to a considerably larger number. The prior schedule though provides a nearly unbiased estimator, there is no clear theoretical evidence showing that this shall work for other situations. The adaptive schedule, without any manual calibration, can provide a nearly unbiased estimator, even when path-sampling is employed, in addition to potential variance reduction.

Table 5. Bayes factor $B_{2,1}$ estimates of two component PET model. T : Number of distributions in SMC and number of iterations used for inference in PMCMC. N : Number of particles in SMC and number chains in PMCMC. The PMCMC and SMC with $N = 192$ are completely N -way parallelized. SMC with $N = 960$ are $N/5$ -way parallelized. *Italic*: Minimum variance for the same computational cost and the same schedule. **Bold**: Minimum variance for the same computational cost and all schedules

Proposal scales			Manual			Adaptive
Annealing scheme			Prior (5)	Posterior (5)	Adaptive	
T	N	Algorithm	Bayes factor estimates ($\log B_{2,1} \pm \text{SD}$)			
500	30	PMCMC	1.7 ± 0.62	-70.9 ± 525.79		
500	192	SMC2-DS	1.6 ± 0.27	1.3 ± 1.13	1.6 ± 0.20	1.6 ± 0.15
		SMC2-PS	1.6 ± 0.27	-3.9 ± 30.02	1.6 ± 0.20	1.6 ± 0.15
100	960	SMC2-DS	1.6 ± 0.37	0.5 ± 1.55	1.6 ± 0.34	1.6 ± 0.21
		SMC2-PS	1.6 ± 0.37	-13.1 ± 66.30	1.6 ± 0.33	1.6 ± 0.21
5000	30	PMCMC	1.6 ± 0.24	-60.3 ± 198.10		
5000	192	SMC2-DS	1.6 ± 0.10	1.6 ± 0.23	1.6 ± 0.09	1.6 ± 0.05
		SMC2-PS	1.6 ± 0.10	1.3 ± 2.98	1.6 ± 0.09	1.6 ± 0.05
1000	960	SMC2-DS	1.6 ± 0.09	1.6 ± 0.33	1.6 ± 0.08	1.6 ± 0.04
		SMC2-PS	1.6 ± 0.09	-0.2 ± 6.63	1.6 ± 0.08	1.6 ± 0.04

Table 6. Path sampling estimator of marginal likelihood of two component PET model. The estimator was approximated using samples from SMC2 algorithm with 1000 particles and 20 iterations, with different numerical integration strategies. Large sample result (see Table 4) provide an estimate of -39.2

Integration rule	Number of grid points (compared to sampled iterations)			
	$\times 1$	$\times 2$	$\times 4$	$\times 8$
Trapezoid	-52.2 ± 5.01	-45.5 ± 1.93	-42.1 ± 1.21	-40.5 ± 1.06
Simpson	-43.2 ± 1.39	-41.0 ± 1.10	-40.0 ± 1.04	-39.4 ± 1.04
Simpson 3/8	-42.1 ± 1.21	-40.5 ± 1.06	-39.7 ± 1.04	-39.3 ± 1.04
Boole	-40.9 ± 1.09	-39.9 ± 1.04	-39.4 ± 1.04	-39.2 ± 1.05

Bias Reduction for Path Sampling Estimator. As seen in Tables 4 and 5, a bad choice of schedule $\alpha(t/T)$ can results in considerable bias for the basic path sampling estimator, here for SMC2-PS but the problem is independent of the mechanism by which the samples are obtained. Increasing the number of iterations can reduce this bias but at the cost of additional computation time. As outlined in Section 3.3.1, in the case of the SMC algorithms discussed here, it is possible to reduce the bias without increasing computational cost significantly. To demonstrate the bias reduction effect, we constructed SMC sampler for the above PET example with only 1000 particles and about 20 iterations specified using the CESS-based adaptive strategy. The path sampling estimator was approximated using Equation (3.13) as well as other higher order numerical integration or by integrating over a grid that contains $\{\alpha_i\}$ at which the samples was generated. The results are shown in Table 6.

Real Data Results. Finally, the methodology of SMC2-PS was applied to measured positron emission tomography data using the same compartmental setup as in the simulations. The data shown in Figure 2 come from a study into opioid receptor density in Epilepsy, with the data being described in detail by Jiang, Aston, and Wang (2009). It is expected that there will be considerable spatial smoothness to the estimates of the volume of distribution, as this is in line with the biology of the system being somewhat regional. Some regions will have much higher receptor density while others will be much lower, yielding higher and lower values of the volume of distribution, respectively. While we did not impose any spatial smoothness but rather estimated the parameters independently for each time series at each spatial location, as can be seen, smooth spatial estimates of the volume of distribution consistent with neurological understanding were found using the approach. This method is computationally feasible for the entire brain on a voxel-by-voxel basis, due to the ease of parallelization of the SMC algorithm. In the analysis performed here, 1000 particles were used, along with an adaptive schedule using a constant $\text{CESS}^I = 0.999$, resulting in about 180 to 200 intermediate distributions. The model selection results are very close to those obtained by a previous study of the same data (Zhou, Aston, and Johansen 2013), although the present approach requires much less implementation effort and has roughly the same computational cost.

4.3 SUMMARY

These two illustrative applications and the GMM example in the supplementary material have essentially shown three aspects of using SMC as a generic tool for Bayesian model

selection. First, as seen in the GMM example, all the different variants of SMC proposed, including both direct and path sampling versions, produce results that are competitive with other model selection methods such as RJMCMC and PMCMC. In addition, in this somewhat simple example, SMC2 performs well, and leads to low variance estimates with no appreciable bias. The effect of adaptation was studied more carefully in the nonlinear ODE example, and it was shown that using both adaptive selection of distributions as well as adaptive proposal variances leads to very competitive algorithms, even against those with significant manual tuning. This suggests that an automatic process of model selection using SMC2 is possible. In the final example, considering the easy parallelization of algorithms such as SMC2 suggests that great gains in variance estimation can be made using settings such as GPU computing for application where computational resources are of particular importance (such as in image analysis as in the PET example). It is also clear that the negligible cost of the bias reduction techniques described means that one should always consider using these to reduce the bias inherent in path sampling estimation. As can also be seen in the supplementary material, there is theoretical justification, in terms of a central limit theorem, available for the path sampling estimator considered in SMC2-PS.

5. DISCUSSION

It has been shown that SMC is an effective Monte Carlo method for Bayesian inference for the purpose of model comparison. Three approaches have been outlined and investigated in several challenging scenarios. The proposed strategy is always competitive and often substantially outperforms the state of the art in this area.

Among the three approaches developed, SMC1 is applicable to very general settings. It can provide a robust alternative to RJMCMC when inference on a countable collection of models is required (and could be readily combined with the approach of Jasra et al. (2008) at the expense of a little additional implementation effort). However, like all Monte Carlo methods involving between model moves, it can be difficult to design efficient algorithms in practice. The SMC3 algorithm is conceptually appealing. However, specifying a suitable sequence of distributions between two posterior distributions is challenging.

The SMC2 algorithm, which only involves within-model simulation, is most straightforward to implement in many interesting problems and has been shown to be exceedingly robust in many settings. As it depends largely upon a collection of within-model MCMC moves, any existing MCMC algorithms can be reused in the SMC2 framework. However, much less tuning is required because the algorithm is fundamentally less sensitive to the mixing of the Markov kernel and it is possible to implement effective adaptive strategies at little computational cost. With adaptive placement of the intermediate distributions and specification of the MCMC kernel proposals, it provides a robust and nearly automatic model comparison method.

Compared to the PMCMC algorithm, SMC2 has greater flexibility in the specification of distributions. Unlike PMCMC, where the number and placement of distributions can affect the mixing speed and hence performance considerably, increasing the number of distributions will always benefit a SMC sampler given the same number of particles. Compared

to its no-resampling variant, it has been shown that SMC samplers with resampling can reduce the variance of normalizing constant estimates considerably.

Even after three decades of intensive development, no Monte Carlo method can solve the Bayesian model comparison problem completely automatically without any manual tuning. However, SMC algorithms and the adaptive strategies demonstrated in this article show that even for realistic, interesting problems, these samplers can provide good results with very minimal tuning and few design difficulties. For many applications, they could already be used as near automatic, robust solutions. For more challenging problems, they can serve as solid foundation for the design of dedicated algorithms.

SUPPLEMENTARY MATERIALS

The file Zhouetal_supp.pdf (PDF file) provides:

Additional examples: A Gaussian mixture model example used to compare all algorithms considered in this article and additional results for the PET model.

Technical Material: A derivation of the conditional ESS and a central limit theorem for the path sampling estimator suggested in the methodology section.

The file vSMC.zip (zip file) provides the code to analyze the simulated examples in the article.

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